Are Th-doped Y_2C_3 and La_2C_3 two-band superconductors?

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Abstract

The superconducting sesquicarbides R_2C_3 have noncentrosymmetric point group symmetry T_d. Spin-orbit coupling lifts the spin degeneracy of electronic bands in the most of the Brillouin zone. Nevertheless, due to high symmetry, there are a few directions along which the Fermi surfaces must touch. This leads to two-band effects in the superconducting state.

Key words: Two-band superconductivity, sesquicarbides

The recent discovery of heavy-fermion superconductivity in the noncentrosymmetric tetragonal compound $CePt_3Si$ [1] has raised a new challenge concerning the nature of superconducting states [2,3]. This is due to the lifting of spin degeneracy of electronic bands in noncentrosymmetric crystals by strong spin-orbit coupling (SOC). This note is devoted to two series of compounds with so-called sesquicarbide structure, $(Y_{1-x}Th_x)_2C_{3-y}$ and $(La_{1-x}Th_x)_2C_{3-y}$, discovered more than three decades ago [4,5]. The crystals appeared to be superconducting with T_c up to 17 K. The sesquicarbides have space group $I\bar{4}3d$ [6], which belongs to the tetrahedral crystallographic class T_d. Centres of symmetry are therefore absent from the structure. Th doping (x can reach 0.9) introduces two features which make the sesquicarbides similar to $CePt_3Si$, namely Th has the same number of f-electrons in the outer shell as Ce, and also one can expect strong SOC effects. Unfortunately, the physical properties of the sesquicabides have not been studied systematically so far.

Here I predict that superconductivity in Th-doped sesquicarbides should involve at least two bands with possibly different magnitudes of the superconducting gap. If the Fermi surfaces corresponding to different bands split by strong SOC are separated, a one-band treatment may be sufficient [3]. For $(Y_{1-x}Th_x)_2C_{3-y}$ and $(La_{1-x}Th_x)_2C_{3-y}$, there are directions in the Brillouin zone where the SOC split Fermi surfaces must touch. This is clear from the following group theoretical argument. The electronic states are described by the Bloch spinors

$$\Psi^{\pm}_{\mathbf{k}}(\mathbf{r}) = U^{\pm}_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{kr}}, \quad U^{\pm}_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{2V}} \begin{pmatrix} u_{\mathbf{k},\uparrow} \\ u^{\pm}_{\mathbf{k},\downarrow} \end{pmatrix}, \quad (1)$$

where $\mathbf{k}$ is quasimomentum, V is the sample volume and indexes $\pm$ refer to the two SOC split bands [3]. Just as in the case of zero SOC, the functions $U^{\pm}_{\mathbf{k}}(\mathbf{r})$ span irreducible representations of the point group which leaves the vector $\mathbf{k}$ invariant. However, in the present case the representations are double valued since $U^{\pm}_{\mathbf{k}}(\mathbf{r})$ describe spin-$\frac{1}{2}$ particles. For T_d symmetry, the vectors $\mathbf{k}_1 = (k_x, 0, 0), (0, k_y, 0), (0, 0, k_z)$ are invariant under the group $C_{2v} \subset T_d$. This group has only one double valued irreducible representation, which is two-dimensional. [2] Hence, there must be two linearly independent solutions of the Schrödinger equation corresponding to each allowed energy value $\varepsilon_{\mathbf{k}_1}$.

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[2] Note that one-dimensional representations should not be combined with their complex conjugate since time reversal changes the sign of $\mathbf{k}$.

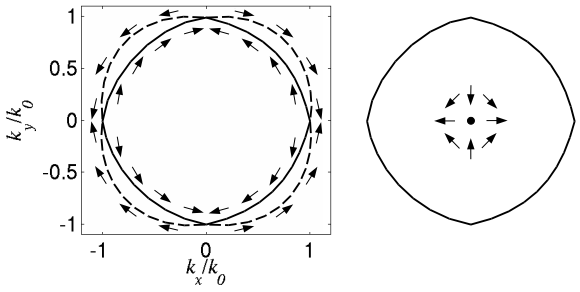

Fig. 1. *Left.* Cross section of the Fermi surfaces by the plane $k_z = 0$. Solid line corresponds to the '+' band, dashed line – the '-' band. Arrows denote the direction of spin. *Right.* Spins in the '+' band around a node of $\boldsymbol{g}_{\mathbf{k}}$.

For the sake of simplicity, I further proceed with addressing the effects of SOC by the perturbative approach proposed in [2]. The single particle Hamiltonian is approximated by

$$H_1 = \sum_{\mathbf{k},s} \varepsilon^0_{\mathbf{k}} c^\dagger_{\mathbf{k}s} c_{\mathbf{k}s} + \alpha \sum_{\mathbf{k},s,s'} \boldsymbol{g}_{\mathbf{k}} \boldsymbol{\sigma}_{ss'} c^\dagger_{\mathbf{k}s} c_{\mathbf{k}s'}, \qquad (2)$$

where $\alpha > 0$ is constant, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices and the vector $\boldsymbol{g}_{\mathbf{k}} = [g_x(\mathbf{k}), g_y(\mathbf{k}), g_z(\mathbf{k})]$ is chosen such that $\boldsymbol{g}_{\mathbf{k}}\boldsymbol{\sigma}$ reduces the symmetry of H_1 from $G \otimes I$ to G, the actual point group. Here I is inversion. The Hamiltonian (2) is diagonalized by the two spinors (1) with

$$u^\pm_{\mathbf{k},\downarrow}/u_{\mathbf{k},\uparrow} = (\pm|\boldsymbol{g}_{\mathbf{k}}| - g_z)/(g_x - ig_y), \qquad (3)$$

corresponding to the eigenvalues

$$\varepsilon^\pm_{\mathbf{k}} = \varepsilon^0_{\mathbf{k}} \pm \alpha|\boldsymbol{g}_{\mathbf{k}}|. \qquad (4)$$

It is a somewhat lengthy but straightforward algebraic exercise to show that

$$\mathbf{s}^\pm_{\mathbf{k}} \equiv \frac{\hbar}{2}\langle\Psi^\pm_{\mathbf{k}}|\boldsymbol{\sigma}|\Psi^\pm_{\mathbf{k}}\rangle = \pm\frac{\hbar}{2}\frac{\boldsymbol{g}_{\mathbf{k}}}{|\boldsymbol{g}_{\mathbf{k}}|}. \qquad (5)$$

Hence, $\boldsymbol{g}_{\mathbf{k}}$ defines the direction of spin $\mathbf{s}^\pm_{\mathbf{k}}$ carried by particles in both bands.

For $G = T_d$, $G \otimes I = O_h$, and $\boldsymbol{g}_{\mathbf{k}}\boldsymbol{\sigma}$ transforms according to the representation A_{2u} of O_h. Namely,

$$\boldsymbol{g}_{\mathbf{k}} = [k_x(k_z^2 - k_y^2), k_y(k_x^2 - k_z^2), k_z(k_y^2 - k_x^2)] \qquad (6)$$

It follows from (5) that the points $\boldsymbol{g}_{\mathbf{k}} = 0$, where the Fermi surfaces touch, are singular, *i. e.* the direction of spin is not defined. This is essentially because the spin quantization axis can be chosen arbitrary for spin degenerate states. A cross section of the Fermi surfaces corresponding to (6) is shown in Fig. 1 together with the spin structure. It is assumed that the "unperturbed" Fermi surface is spherical, $\varepsilon^0_{\mathbf{k}} = \hbar^2 k_0^2/2m$.

Finally, I consider the pairing interaction term H_2 in the Hamiltonian, which leads to the formation of the superconducting state. I assume that before SOC has been turned on, the electrons were paired in a singlet superconducting state, with the order parameter $\psi(\mathbf{k})$. Within the weak coupling approach,

$$H_2 = \frac{1}{2}\sum_{\mathbf{k}} \psi(\mathbf{k})(c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - c^\dagger_{\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\uparrow}) + \text{h.c.} \qquad (7)$$

If by some reason it is desirable, one can start with a triplet pairing state. As far as the symmetry of the superconducting state is concerned, the result will be essentially the same [3].

Equation (7) is valid for the degenerate states at the nodes of $\boldsymbol{g}_{\mathbf{k}}$. However, for the rest of the Brillouin zone H_2 should be expressed in terms of the new fermion operators $c^\dagger_{\mathbf{k}+}$, $c^\dagger_{\mathbf{k}-}$ corresponding to the bands (4). I introduce the spherical coordinate system $k_x = \cos\theta$, $k_z = \sin\theta\cos\phi$, $k_y = \sin\theta\sin\phi$ and consider the states in the vicinity of $\mathbf{k}_1 = (k_x, 0, 0)$. Then using (3), I obtain

$$\begin{aligned} c^\dagger_{\mathbf{k}\uparrow} &= c^\dagger_{\mathbf{k}+}\sin(\phi/2) + c^\dagger_{\mathbf{k}-}\cos(\phi/2), \\ c^\dagger_{\mathbf{k}\downarrow} &= -ic^\dagger_{\mathbf{k}+}\cos(\phi/2) + ic^\dagger_{\mathbf{k}-}\sin(\phi/2). \end{aligned} \qquad (8)$$

Hence, the pairing interaction is

$$H_2 = \frac{i}{2}\sum_{\mathbf{k}} \psi(\mathbf{k})(c^\dagger_{\mathbf{k}+} c^\dagger_{-\mathbf{k}+} + c^\dagger_{\mathbf{k}-} c^\dagger_{-\mathbf{k}-}) + \text{h.c.} \qquad (9)$$

The factor i is the additional phase factor $t(\mathbf{k})$ which is acquired by the gap function in the superconductors with SOC split bands [3]. Generally, $t(\mathbf{k})$ is an odd function, which follows from the anticommutation of the fermion operators. Equation (9) is written for $\mathbf{k}$ with $\theta \approx 0$, and one cannot replace $\mathbf{k}$ with $-\mathbf{k}$ in the sum. For $\theta \approx \pi$, the right hand side in (9) changes its sign, and thus the oddness of $t(\mathbf{k})$ is restored.

Hence, even though there is no interband coupling terms in (9), the pairing in the two bands is governed by the same order parameter $\psi(\mathbf{k})$, that is both gaps open at the same T_c. However, since $\psi(\mathbf{k})$ at least depends on the absolute value of $\mathbf{k}$, the amplitudes of the gaps away from the nodes of $\boldsymbol{g}_{\mathbf{k}}$ may be quite different, similar to the situation in MgB_2 [7].

In conclusion, it is shown that the Fermi surfaces of $(Y_{1-x}Th_x)_2C_{3-y}$ and $(La_{1-x}Th_x)_2C_{3-y}$ that are split by SOC must touch along some directions in the Brillouin zone due to their high crystallographic symmetry. This implies that the minimal model should at least include two bands with the superconducting gaps opening at the same T_c. I hope that this note will stimulate interest towards a more active investigation of the non-trivial superconducting properties of Th-doped sesquicarbides.

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